

An intrinsic connection between topological stabilities of Fermi surfaces and topological insulators/superconductors

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An intrinsic connection between the topological stabilities of Fermi surfaces and topological insulators/superconductors is revealed. Based on our rigorous theory for topological stabilities of all types of Fermi surfaces, we strictly derive a quantitative relation between the topological types of Fermi surfaces and topological insulators/superconductors, producing exactly a complete table of topological types for all insulators/superconductors. In particular, we establish a general index theorem relating the topological charge of Fermi surfaces on the natural boundary of a strong topological insulator/superconductor to its bulk topological number. The implications of the general index theorem on the boundary quasi-particles are also addressed briefly.

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As is known from quantum mechanics, all symmetries have either the unitary or anti-unitary presentations[1]. While unitary ones are various, such as translation symmetry and rotation symmetry *etc.*, there are only two kinds of anti-unitary symmetries, *i.e.* the time-reversal symmetry(TRS) and particle-hole symmetry(PHS). For a condensed matter system with Hamiltonian $\mathcal{H}(\mathbf{k})$, they can be respectively represented as

$$\begin{cases} T^\dagger \mathcal{H}(\mathbf{k}) T = \mathcal{H}^T(-\mathbf{k}), T = \eta_T T^T & (\text{TRS}) \\ C^\dagger \mathcal{H}(\mathbf{k}) C = -\mathcal{H}^T(-\mathbf{k}), C = \eta_C C^T & (\text{PHS}) \end{cases},$$

where T and C are unitary matrices, and either η_C or η_T is equal to ± 1 . We know that disorders are ubiquitous in condensed matter systems, and usually only TRS and PHS can be preserved by disorders. Thus in the random matrix theory, all Hamiltonians are classified by considering TRS and PHS[2–4]. It is easy to verify that $\{CT^\dagger, \mathcal{H}\} = 0$, which implies CT^\dagger is a chiral symmetry(CS)[5]. So to obtain a complete classification, it is necessary to include a CS. As a result, either TRS or PHS may take three possible types ($\eta = \pm 1$ and absent), and therefore there are nine classes. In addition, considering that the chiral symmetry may be preserved or not when both TRS&PHS are absent, we totally have ten classes, as summarized in Tab.[I], which is the famous Cartan classification[2–4].

A Fermi surface(FS) is a gapless region in the \mathbf{k} -space. Some FSs are stable against disorders/perturbations, while some others are vulnerable and easy to be

gapped[6]. It is found that the topological charge of an FS is responsible for its stability[6–9]. For a $(d - p)$ -dimensional FS in a d -dimensional \mathbf{k} -space, we can choose a p -dimensional sphere S^p from (ω, \mathbf{k}) -space to enclose it in the its transverse dimension, where p is referred to as the codimension of the FS. Note that the spectrum is gapped on the whole S^p since the S^p is constructed in the transverse dimension of an FS. For an FS without any symmetry, *i.e.* in the class A in Tab.[I], its topological charge is given by the homotopy number of the Green's function, $G(\omega, \mathbf{k}) = [i\omega - \mathcal{H}(\mathbf{k})]^{-1}$, restricted on the S^p [6–8]. This idea is generalized to FSs for the other classes for characterizing the corresponding types of symmetry-dependent topological charges in terms of the Green's function[9], as summarized in Tab.[II] (from a left-to-right manner), where only eight classes with either TRS or PHS are listed since the classes A and AIII are not closely relevant to a main purpose of this paper. The key idea is that for a $\mathcal{H}(\mathbf{k})$ with either TRS or PHS, the symmetries can be preserved on the S^p if it is chosen to be centrosymmetric with respect to the origin of (ω, \mathbf{k}) -space as illustrated in Fig(1). Then on the S^p in a symmetry class, we can define topological charges for the corresponding symmetries. In Ref.[9], all six types of topological charges are explicitly given with mathematical expressions, among which three ones are belong to the non-chiral cases while the other three ones correspond to the chiral cases. In Tab.[II], the \mathbf{Z} , $\mathbf{Z}_2^{(1)}$, and $\mathbf{Z}_2^{(2)}$ denote the integer-valued topological charge, \mathbf{Z}_2 -valued topological charge for the first descent of a \mathbf{Z} -type, and \mathbf{Z}_2 -valued topological charge for the second descent of a \mathbf{Z} -type. Notably, it can be seen from Tab.[II] (from a left-to-right manner) that there exists an eight-fold periodicity:

$$K_{FS}(p, i) = K_{FS}(p + n, i + n), \quad (1)$$

where $K_{FS}(p, i)$ denotes the item of i th row and p th column in Tab.[II], and i and p are integers of modular 8. Here the choice of capital letter 'K' may imply that this

	Non-chiral case					Chiral case				
	A	AI	D	AII	C	AIII	BDI	DIII	CII	CI
T	0	+1	0	-1	0	0	+1	-1	-1	-1
C	0	0	+1	0	-1	0	+1	+1	-1	+1
S	0	0	0	0	0	1	1	1	1	1

TABLE I: Hamiltonian Classification

$p \backslash i$	AI	BDI	D	DIII	AII	CII	C	CI	i/D
	1	2	3	4	5	6	7	8	
0	0	Z	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	2Z	0	0	2
1	0	0	Z	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	2Z	0	3
2	0	0	0	Z	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	2Z	4
3	2Z	0	0	0	Z	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	5
4	0	2Z	0	0	0	Z	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	6
5	$\mathbf{Z}_2^{(2)}$	0	2Z	0	0	0	Z	$\mathbf{Z}_2^{(1)}$	7
6	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	2Z	0	0	0	Z	8
7	Z	$\mathbf{Z}_2^{(1)}$	$\mathbf{Z}_2^{(2)}$	0	2Z	0	0	0	9
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\vdots

TABLE II: Periodic Table for FSs and TIs/TSCs[9]. i is the index of symmetry classes, p is the codimension of an FS, and D is the space-time dimension of a TI/TSC.

eight-fold periodicity is connected to the K-theory[10–12].

A strong topological insulator(TI) /superconductor(TSC) has gapless boundary modes, which are robust against disorders, and protected by its nontrivial bulk topological number[13–15]. It is crucial to observe that all six formulas for the topological charges of FSs can also be used to calculate the topological numbers of TIs/TSCs, where, in stead of making the integration over S^p for an FS, we make it over the whole (ω, \mathbf{k}) -space in these formulas[14, 16–18]. This will be illustrated later around Eq.(7) and Eq.(10). A naive intuition were that the whole (ω, \mathbf{k}) -space for a TI/TSC in a symmetry class when being regarded as an S^D could be equivalent to an S^p enclosing an FS with codimension $p = D$ (here $D = d + 1$ denotes the total space-time dimension of a TI/TSC) with the same symmetry class in its transverse dimension, and we would obtain a same periodic table for TIs/TSCs just by treating p as D . However, the operation of TRS or PHS in the \mathbf{k} -space for a TI/TSC has an intrinsic difference from that for a chosen S^p , as illustrated in Fig.[1]. We first present the result, with relatively technical details of this difference being elaborated later. It turns out that the resulting periodic table for TIs/TSCs is globally shifted from that for the codimension of FSs by two dimensions, *i.e.*,

$$K_{TI}(D, i) = K_{FS}(D - 2, i), \quad (2)$$

where K_{TI} denotes the topological types in the corresponding table of TIs/TSCs. Thus the periodic table for TIs/TSCs can be produced exactly, as illustrated in Tab.[II] (from a right-to-left manner). Combining Eq.(2) with Eq.(1) yields also

$$K_{TI}(D, i) = K_{TI}(D + n, i + n). \quad (3)$$

The periodic table for TIs/TSCs was first postulated by generalizing Pruiskein's theory for the integer quantum hall effect(IQHE)(in the class A) to the other sym-

metry classes[19–22]. The Pruiskein's theory is a non-linear σ model handling disorders, and attributes the stability of the gapless boundary modes against disorders to a topological WZ-term on the boundary[19, 23]. As a specific symmetry class has a unique group for its non-linear sigma model[2–4], the classification in Tab[II] was postulated according to whether eligible topological terms can appear on the boundary of a system in each case[24]. While in the present, it is shown that all the bulk topological numbers are just those (with one-to-one correspondence) for topological charges of FSs identified in Ref.[9]; secondly, the periodic table for TIs/TSCs is refined by classifying the two types of $\mathbf{Z}_2^{(1,2)}$, noting that no such distinction can be seen from the previously postulated table[20–22].

The seemingly accidental two-dimension shifting in Tab.[II], *i.e.* Eq.(2), actually has a natural physical origin embodying the boundary-bulk correspondence of TIs/TSCs. It is known that the boundary gapless modes of a TI/TSC with a given symmetry class are robust against disorders/perturbations that do not break the corresponding symmetry. This implies that the FSs corresponding to these gapless modes must be protected by nontrivial topological charge in the same class according to our theory of topological stable FSs[9]. For concreteness, let us consider a D -dimensional TI/TSC with a symmetry class i that has a $(D - 1)$ -dimensional boundary on the x -direction and a nontrivial topological number $N(D, i)$ in Tab.[II], which leads to a topologically stable gap in the bulk. Under the natural boundary condition of a TI/TSC, *i.e.* no dramatic anisotropy being induced when the system approaches its boundary, FSs on the boundary will always be some Fermi points (or at least some localized manifolds in the \mathbf{k} -space of the boundary which can be continuously deformed to points), which implies that FSs on this TI/TSC's boundary have codimension $p = D - 2$. If requiring the same i th symmetry of the bulk to be preserved on the boundary, we can always choose a large-enough S^{D-2} to enclose all the FSs in the $(D - 1)$ -dimensional (ω, \mathbf{k}) -space of the boundary, such that the symmetry is also preserved on the S^{D-2} . On this S^{D-2} , we can calculate the total topological charge $\nu(D - 2, i)$ of the all FSs on the boundary. Therefore, from Eq.(2), we can yield a general index theorem for the boundary-bulk correspondence of the same system:

$$\nu(D - 2, i) = N(D, i). \quad (4)$$

This general index theorem is a quantitative description of the boundary-bulk correspondence of the all eight classes of TIs/TSCs with either TRS and/or PHS, implying that the nontrivial bulk topology of a TI/TSC is also reflected by its topological charge of the boundary FSs. In other words, for a TI/STC, the same topological origin protects both the stability of FSs on the boundary and the gapped spectrum in the bulk against dis-

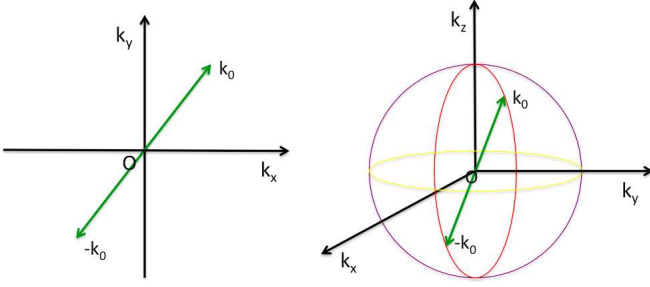


FIG. 1: Symmetry Identification. The left corresponds to a two-dimensional \mathbf{k} -space, and the right corresponds to an S^2 enclosing a Fermi point in a three-dimensional \mathbf{k} -space.

orders/perturbations. We also note that the index theorem for the class A (without any symmetry) has been given in Ref.[6] previously, and rigorously proved in several models[25, 26]. Although the topological charge of FSs in the class A is not explicitly used, it can also be expressed in the form of Eq.(4). Based on the index theorem of the class A, it is obvious that the index theorem is also valid for the class AIII.

We now turn to the detailed derivation of Eq.(2). Although $\mathcal{H}(\mathbf{k})$ and $\mathcal{H}(\mathbf{k})|_{S^{p-1}}$ have the same TRS or PHS, an essential difference lies in that the central point O is in the domain for $\mathcal{H}(\mathbf{k})$, *i.e.* the whole \mathbf{k} -space, while O is outside the chosen S^{p-1} for $\mathcal{H}(\mathbf{k})|_{S^{p-1}}$, with a two-dimensional example being illustrated in Fig.(1). This difference may be viewed as follows. Since TRS or PHS relates a point \mathbf{k}_0 to $-\mathbf{k}_0$, there are invariant points in the whole \mathbf{k} -space, while on an S^{p-1} every point is mapped to another point. It can also be seen from a topological viewpoint. After we compactify a $(p-1)$ -dimensional \mathbf{k} -space to an S^{p-1} by treating the infinity or the boundary of first Brillouin zone as one point, the quotient space resulting from identifying \mathbf{k}_0 with $-\mathbf{k}_0$ in the \mathbf{k} -space is different from that resulting from a chosen S^{p-1} for an FS under the same identification in a higher dimensional \mathbf{k} -space. The latter one is a $(p-1)$ -dimensional real projective space $\mathbb{RP}(p-1)$ [27]. Actually, this difference indeed exists in the analysis of the relation of topological numbers with TRS or PHS. In practical calculations, we use the following spherical coordinates for the chosen S^{p-1} ,

$$\begin{cases} k_1 = \cos s_1 \\ k_2 = \sin s_1 \cos s_2 \\ k_3 = \sin s_1 \sin s_2 \cos s_3 \\ \vdots \\ k_{p-1} = \sin s_1 \sin s_2 \cdots \sin s_{p-2} \cos s_{p-1} \\ k_p = \sin s_1 \sin s_2 \cdots \sin s_{p-2} \sin s_{p-1} \end{cases}$$

with $s_i \in [0, \pi]$ for $i = 1, 2, \dots, p-2$ and $s_{p-1} \in [0, 2\pi)$. Without loss of generality, we have assumed that the FS is a Fermi point with codimension p in a $(p+1)$ -

dimensional (ω, \mathbf{k}) -space. In the following, we focus on the class AII as an illustration, which has only TRS with $\eta_T = -1$, while other seven classes can be greatly in the same way with the same result. The TRS on the chosen S^{p-1} with the spherical coordinates can be represented as

$$T^\dagger \mathcal{H}(s) T = \mathcal{H}^T(\pi - s_1, \dots, \pi - s_{p-2}, \pi + s_{p-1}).$$

Note that the transformation of s_{p-1} is different from those of the others. Correspondingly for Green's function $G(\omega, \mathbf{k}) = [i\omega - \mathcal{H}(\mathbf{k})]^{-1}$, we have

$$T^\dagger G(\omega, s) T = G^T(\omega, \pi - s_1, \dots, \pi - s_{p-2}, \pi + s_{p-1}). \quad (5)$$

While the Green's function for a TI in the class AII satisfies

$$T^\dagger G(\omega, \mathbf{k}) T = G^T(\omega, -\mathbf{k}). \quad (6)$$

We can see that all momentum components of the TI reverse signs under the TRS transformation, which is in contrast to the situation of the chosen S^{p-1} enclosing an FS where the last coordinate s_{p-1} does not reverse its sign. This distinction affects the evaluation of the \mathbf{Z} -type topological number/charge with TRS. We first illustrate how TRS makes the \mathbf{Z} -type topological charge of an FS with codimension $p = 4m+1$ vanish. The formula for the \mathbf{Z} -type topological charge with codimension $p = 2n+1$ is given by

$$\begin{aligned} & \nu(2n+1, 5) \\ &= C_{2n+1} \int_{S^p} d\omega d^{2n} s \epsilon^{\mu_1 \mu_2 \cdots \mu_{2n+1}} \\ & \quad \text{tr} (G \partial_{\mu_1} G^{-1} G \partial_{\mu_2} G^{-1} \cdots G \partial_{\mu_{2n+1}} G^{-1}(\omega, s)), \end{aligned} \quad (7)$$

where $C_{2n+1} = -n!/(2n+1)!(2\pi i)^{n+1}$. Implementing the TRS transformation, *i.e.* Eq.(5), and the coordinate substitution $s'_i = \pi - s_i$ with $i = 1, 2, \dots, 2n-1$ and $s'_{2n} = \pi + s_{2n}$, we have

$$\begin{aligned} & \nu(2n+1, 5) \\ &= -C_{2n+1} \int_{S^p} d\omega d^{2n} s' \epsilon^{\mu'_1 \mu'_2 \cdots \mu'_{2n+1}} \\ & \quad \text{tr} (G^T \partial_{\mu'_1} G^{T-1} \cdots G^T \partial_{\mu'_{2n+1}} G^{T-1}(\omega, s')) \\ &= C_{2n+1} \int_{S^p} d\omega d^{2n} s \epsilon^{\mu_1 \mu_2 \cdots \mu_{2n+1}} \\ & \quad \text{tr} (G \partial_{\mu_{2n+1}} G^{-1} G \partial_{\mu_{2n}} G^{-1} \cdots G \partial_{\mu_1} G^{-1}(\omega, s)). \end{aligned} \quad (8)$$

Making a permutation that reverses the order of all the indices of ϵ , we obtain

$$\nu(2n+1, 5) = (-1)^{n-1} \nu(2n+1, 5), \quad (9)$$

where the extra $(-1)^n$ comes from the permutation. Now it is clear that when $n = 2m$ with m being an integer,

i.e. $p = 4m + 1$, the \mathbf{Z} -type topological charge of an FS is vanished for the class AII. When handling the TRS of minus sign (the Class AII) for a TI, the process is almost the same. First, the integral form of topological number is the same as Eq.(7), but the integration is made over the whole (ω, \mathbf{k}) -space, rather than over S^p ,

$$\begin{aligned} & N(2n + 1, 5) \\ &= C_{2n+1} \int d\omega d^{2n}k \epsilon^{\mu_1 \mu_2 \dots \mu_{2n+1}} \\ & \text{tr} (G \partial_{\mu_1} G^{-1} G \partial_{\mu_2} G^{-1} \dots G \partial_{\mu_{2n+1}} G^{-1}(\omega, \mathbf{k})) \end{aligned} \quad (10)$$

In a similar way to the case of FS, we make the variable substitution $\mathbf{k}' = -\mathbf{k}$, matrix transposition, and then a permutation of reversing all the indices of ϵ . The only difference is that when substituting the variables, we could not obtain an extra minus sign as that in second first equality of Eq.(8), since the number of partial derivatives of k_i is even. Thus we have

$$N(2n + 1, 5) = (-1)^n N(2n + 1, 5), \quad (11)$$

which implies the topological number for a TI of $D = 4m + 3$ in the class AII is always trivial, but that of $D = 4m + 1$ can be nontrivial.

Comparing Eq.(9) with Eq.(11), we see clearly a two-dimension shifting from $K_{FS}(p, 5)$ to $K_{TI}(D, 5)$ [28]. The same result is obtained for the other seven classes due to the same reason. Thus it is rather clear at present that the two-dimension shifting, *i.e.* Eq.(2) reflects the topological difference between the \mathbf{k} -space and the chosen S^{p-1} to enclose an FS with the symmetry class being considered.

The index theorem of Eq.(4), as a quantitative relation, has strong predictions on the low-energy effective theories for the boundaries of TIs, as it is known that the topological charge of an FS can determine the quasi-particle types emergent from the FS[6–8, 18]. Based on the Atiyah-Bott-Singer(ABS) construction in K-theory, quasi-particles emergent from an FS of unit \mathbf{Z} -type topological charge in a non-chiral class in Tab.[I] have to be Dirac fermions of Weyl-type[8, 12, 29]:

$$\mathcal{H}_W = \pm \sum_{i=1}^{2n+1} k_i \Gamma_{(2n+1)}^i, \quad (12)$$

where $\Gamma_{(2n+1)}^i$ are $2^n \times 2^n$ matrices satisfy Clifford Algebra[30], \pm corresponds to positive/negative unit charge, and the codimension of the FS is $p = 2n + 1$. As a multiply charged FS can always be perturbed to unit FSs, we see that the typical low-energy effective theory for the boundary of a \mathbf{Z} -type TI in a non-chiral class is a collection of Weyl-type Hamiltonians with either positive or negative unit topological charge satisfying that the total topological charge being the bulk topological number. For an FS of unit \mathbf{Z} -type topological charge in a chiral

class in Tab.[I], the ABS construction also determines the quasi-particles emergent from the FS are Dirac fermions in the following form[18]:

$$\mathcal{H}_D = \pm k_1 \Gamma_{(2n+1)}^1 + \sum_{i=2}^{2n} k_i \Gamma_{(2n+1)}^i, \quad (13)$$

where \pm corresponds to positive/negative unit charge. With the chiral symmetry being preserved on the boundary, the index theorem implies that the typical low-energy effective theory for the boundary of a \mathbf{Z} -type TI in a chiral class is a collection of Hamiltonians in the form of Eq.(13) with positive/negative unit charge satisfying that the total topological charge is the bulk topological number. Actually our theory can be illustrated by the famous lattice Dirac model of $D = 5$ in the class AII[16, 31], where the boundary low-energy theory is a collection of Weyl Hamiltonians, and the number of flavors corresponding to the total topological charge of FSs is equal to the bulk topological number. We also note that for a \mathbf{Z} -type TI with multiple topological numbers, Dirac particles with non-linear dispersion relations may exist on its boundary, but only under some special boundary conditions[6, 7, 32].

For a nontrivial \mathbf{Z}_2 -type FS, the nontrivial topological charge can only be one. The quasi-particle form may not be uniquely determined, since the ABS construction is not applicable. For instance, both $\mathcal{H} = k_x \sigma_1 + k_y \sigma_2 + \lambda(k_x + k_y) \sigma_3$ and $\mathcal{H} = k_x^3 \sigma_1 + k_y^3 \sigma_2 + \lambda(k_x + k_y)^3 \sigma_3$ have a nontrivial $\mathbf{Z}_2^{(1)}$ -type Fermi point of codimension 2 in the class AII, and are eligible to be the boundary effective theory of a nontrivial three-dimensional TI with TRS in this class. As an example of the second descent $\mathbf{Z}_2^{(2)}$, let us consider a nontrivial two-dimensional TI in the class AII, *i.e.* the quantum spin hall system[13, 14]. If the bulk has a nontrivial $\mathbf{Z}_2^{(2)}$ -type topological number, with the same TRS being preserved on the boundary, there exist Fermi points of codimension $p = 1$ in this type with the nontrivial total topological charge, and both $\mathcal{H} = k_x \sigma_3 + \alpha k_x^{(2n+1)} + \beta k_x^{(2m+1)}$ and $\mathcal{H} = k_x^3 \sigma_3 + \alpha k_x^{(2n+1)} + \beta k_x^{(2m+1)}$ are eligible to be the boundary effective theory. Although the prediction from \mathbf{Z}_2 -type cases is not as strong as that of \mathbf{Z} -type cases, we can still exclude boundary models with only FSs of trivial \mathbf{Z}_2 -type charge. For instance, although $\mathcal{H} = k_x^2 \sigma_2 \otimes \sigma_3 + k_y^2 \sigma_2 \otimes \sigma_1$ has the TRS with $T = \mathbf{1} \otimes \sigma_2$ satisfying $T^T = -T$, it cannot be the boundary effective theory of a nontrivial TI in the class AII with $D = 4$, as its FS has a trivial topological charge. In general, the exact quasi-particle form on the boundary for a \mathbf{Z}_2 -type TI depends not only on its topological number, but also on concrete models and boundary conditions.

We now have a further understanding of the boundary-bulk correspondence of strong TIs from Eq.(4). Not only the existence of boundary modes is determined by the bulk topology, but also the form of boundary low-energy

effective theory may be predicted and restricted by the bulk topology.

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